PROCEDURE FOR CORRECTING IMAGES FROM SBC DETECTORS
SBC SECTOR 19 BEAMLINES

The following procedure outlines the accepted method for correcting images from the CCD detectors at the SBC Sector 19 beamlines. The computer software that is used to carry out this procedure is part of the *d*trek* package (J. W. Pflugrath, Molecular Structure Corporation). Image acquisition (*dtcollect*), display (*dtdisplay*), averaging (*dtdisplay* and *dtaverage*) and correction (*dtcorrect*) are performed using the current version of *d*trek* used at the SBC. In the case of single-crystal diffraction experiments, the corrected images may then be processed with *d*trek*, *MOSFLM* or other processing software capable of reading corrected images from the SBC CCD detectors. This procedure or parts thereof should be repeated for each data scan, image or group of images to be corrected. Suggestions for and/or problems with this procedure should be reported to Frank Rotella.

1. Acquire the images to be corrected, and note for these images:
   - the exposure time in seconds.
   - the sample-to-detector distance in millimeters.
   - the detector image size — full-frame or 2 × 2-binned.

2. Acquire additional images that will also be needed in the correction procedure:
   - 10 dark images (dark.????) with exposure time and image size identical to that for the images to be corrected.
   - a direct beam image (dirbeam_*DDD*.0001) with a sample-to-detector distance of *DDD* mm, which is identical to that for the images to be corrected.

3. Open an xterm session on one of your assigned Linux computers using your assigned user account.

4. From the Linux xterm session:
   - create a subdirectory ("mkdir Corrected") under the directory containing the images to be corrected.
   - locate your working directory ("cd") at the Corrected subdirectory.

5. Copy the appropriate files and scripts for correcting images to the Corrected subdirectory:
   - execute the script *getcorrect* from the Linux xterm session:
     - *getcorrect* will prompt you for the beamline on which the images to be corrected were collected (valid values are *BM* or *ID*) and the size of the images to be corrected (valid values are *full* or *binned*).
     - otherwise, you may include the beamline and image size parameters on the command line.
     - if either of the beamline or image size parameters is invalid, *getcorrect* terminates with an error message.
     - the files dark_initsd.img, distor.calpar, distor.inv_x_int, distor.inv_y_int, distor.x_int, distor.y_int, dtavdark.com, dtcorrect.com and nonunf for the appropriate beamline and detector image size are copied into the Corrected subdirectory.

6. Produce an averaged, dezingered dark image from the acquired dark images:
   - execute *dtdisplayZ*, where Z is bm or id as appropriate, from the Linux xterm session to produce an "Underlay"ed dark image (dark.und) from the acquired dark images:
     - "File" _ "New" _ "Underlay…" from the *dtdisplay* interface.
     - save dark.und ("File" _ "Save Image As…") in the Corrected subdirectory.
   - create an averaged, dezingered dark image (dark.dtav), standard deviation file (dark.dtsd) and rejects file (dark.0001rejects) by executing the script *dtavdark.com* from the Linux xterm session:
     - if the names of the acquired dark images are different from those prescribed above, edit the script to reflect this (see "set TEMPLATE =" and "set BASE   =").
     - if the number of acquired dark images is different from that prescribed above, edit the script to reflect this (see "set NUM   =").
     - execute the command *dtavdark.com >&! dtavdark.log &*

7. Determine the coordinates of the direct beam position from the image dirbeam_*DDD*.0001 using *dtdisplayZ*, where Z is bm or id as appropriate, from the Linux xterm session:
   - the horizontal coordinate is x.
   - the vertical coordinate is y.
   - measure both coordinates to the nearest 0.1 pixel.

8. Edit the script used to produce corrected images (*dtcorrect.com*) from the Linux xterm session; verify or change the following parameters in the script:
   - -dark ./dark.dtav
   - -distor ./distor
   - -nonunf ./nonunf
   - -beamx *X.X* (*X.X* is the horizontal coordinate of the direct beam position.)
   - -beamy *Y.Y* (*Y.Y* is the vertical coordinate of the direct beam position.)
   - -seq *A B* (*A* is the beginning and *B*, the ending sequence number of the images to be corrected.)
   - -gocorrect "../*filename*.????" "./*filename*_dtcor.????" (*filename* is the template name of the images to be corrected.)
     - the input images (*filename*.????) should be located in the parent directory of the Corrected subdirectory.
     - the output images (*filename*_dtcor.????) will be written in the Corrected subdirectory.
   - -gocorrect ../dirbeam_*DDD*.0001 ./dirbeam_*DDD*_dtcor.0001
     - the input direct beam image (dirbeam_*DDD*.0001) should be located in the parent directory of the Corrected subdirectory.
     - the output direct beam image (dirbeam_*DDD*_dtcor.0001) will be written in the Corrected subdirectory.
     - the coordinates of the direct beam should be redetermined from dirbeam_*DDD*_dtcor.0001 using *dtdisplayZ*, where Z is bm or id as appropriate, to process corrected single-crystal diffraction images using *d*trek*, *MOSFLM*, etc.
   - Further details regarding the program *dtcorrect* and its parameters can be obtained by executing the command *dtcorrect –h*.

9. Execute the *dtcorrect.com* script to correct the desired images from the Linux xterm session:
   - A single 2 × 2-binned image is corrected in about 7 seconds on a 1-GHz computer.
   - A single full-frame image is corrected in about 26 seconds on a 1-GHz computer.